

* * * * * Welcome to STN International * * * * *

NEWS	1			Web Page for STN Seminar Schedule - N. America
NEWS	2	DEC	01	ChemPort single article sales feature unavailable
NEWS	3	JUN	01	CAS REGISTRY Source of Registration (SR) searching enhanced on STN
NEWS	4	JUN	26	NUTRACEUT and PHARMAML no longer updated
NEWS	5	JUN	29	INSCOPROFILE now reloaded monthly
NEWS	6	JUN	29	EPFULL adds Simultaneous Left and Right Truncation (SLART) to AB, MCLM, and TI fields
NEWS	7	JUL	09	PATDPAFULL adds Simultaneous Left and Right Truncation (SLART) to AB, CLM, MCLM, and TI fields
NEWS	8	JUL	14	USGENE enhances coverage of patent sequence location (PSL) data
NEWS	9	JUL	27	CA/CAPlus enhanced with new citing references
NEWS	10	JUL	16	GBFULL adds patent backfile data to 1855
NEWS	11	JUL	21	USGENE adds bibliographic and sequence information
NEWS	12	JUL	28	EPFULL adds first-page images and applicant-cited references
NEWS	13	JUL	28	INPADOCDB and INPAFAMDB add Russian legal status data
NEWS	14	AUG	10	Time limit for inactive STN sessions doubles to 40 minutes
NEWS	15	AUG	18	COMPENDEX indexing changed for the Corporate Source (CS) field
NEWS	16	AUG	24	ENCOMPLIT/ENCOMPLIT2 reloaded and enhanced
NEWS	17	AUG	24	CA/CAPlus enhanced with legal status information for U.S. patents
NEWS	18	SEP	09	50 Millionth Unique Chemical Substance Recorded in CAS REGISTRY
NEWS	19	SEP	11	WPIDS, WPINDEX, and WPIX now include Japanese FTERM thesaurus

NEWS EXPRESS MAY 26 09 CURRENT WINDOWS VERSION IS V8.4,
AND CURRENT DISCOVER FILE IS DATED 06 APRIL 2009.

NEWS HOURS	STN Operating Hours Plus Help Desk Availability
NEWS LOGIN	Welcome Banner and News Items

Enter NEWS followed by the item number or name to see news on that specific topic.

All use of STN is subject to the provisions of the STN customer agreement. This agreement limits use to scientific research. Use for software development or design, implementation of commercial gateways, or use of CAS and STN data in the building of commercial products is prohibited and may result in loss of user privileges and other penalties.

* * * * * STN Columbus * * * * *

FILE 'HOME' ENTERED AT 16:06:05 ON 23 SEP 2009

=> file reg		
COST IN U.S. DOLLARS	SINCE FILE	TOTAL
	ENTRY	SESSION
FULL ESTIMATED COST	0.22	0.22

FILE 'REGISTRY' ENTERED AT 16:06:26 ON 23 SEP 2009
USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.
PLEASE SEE "HELP USAGETERMS" FOR DETAILS.
COPYRIGHT (C) 2009 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file

provided by InfoChem.

STRUCTURE FILE UPDATES: 22 SEP 2009 HIGHEST RN 1186072-05-8
DICTIONARY FILE UPDATES: 22 SEP 2009 HIGHEST RN 1186072-05-8

New CAS Information Use Policies, enter HELP USAGETERMS for details.

TSCA INFORMATION NOW CURRENT THROUGH June 26, 2009.

Please note that search-term pricing does apply when
conducting SmartSELECT searches.

REGISTRY includes numerically searchable data for experimental and
predicted properties as well as tags indicating availability of
experimental property data in the original document. For information
on property searching in REGISTRY, refer to:

<http://www.cas.org/support/stngen/stndoc/properties.html>

=>

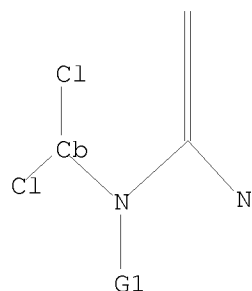
Uploading C:\Program Files\Stnexp\Queries\10531783-broad.str

L1 STRUCTURE UPLOADED

=> d l1

L1 HAS NO ANSWERS

L1 STR



G1 Me,Et,n-Pr,i-Pr

Structure attributes must be viewed using STN Express query preparation.

=> s l1

SAMPLE SEARCH INITIATED 16:06:45 FILE 'REGISTRY'

SAMPLE SCREEN SEARCH COMPLETED - 6241 TO ITERATE

32.0% PROCESSED 2000 ITERATIONS

4 ANSWERS

INCOMPLETE SEARCH (SYSTEM LIMIT EXCEEDED)

SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE **COMPLETE**

BATCH **COMPLETE**

PROJECTED ITERATIONS: 120083 TO 129557

PROJECTED ANSWERS: 38 TO 460

L2 4 SEA SSS SAM L1

=> s l1 full

FULL SEARCH INITIATED 16:06:49 FILE 'REGISTRY'

FULL SCREEN SEARCH COMPLETED - 126827 TO ITERATE

100.0% PROCESSED 126827 ITERATIONS
SEARCH TIME: 00.00.03

248 ANSWERS

L3 248 SEA SSS FUL L1

=> file caplus

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

186.36

186.58

FILE 'CAPLUS' ENTERED AT 16:07:33 ON 23 SEP 2009

USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT.

PLEASE SEE "HELP USAGETERMS" FOR DETAILS.

COPYRIGHT (C) 2009 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 23 Sep 2009 VOL 151 ISS 13

FILE LAST UPDATED: 22 Sep 2009 (20090922/ED)

REVISED CLASS FIELDS (/NCL) LAST RELOADED: Jun 2009

USPTO MANUAL OF CLASSIFICATIONS THESAURUS ISSUE DATE: Jun 2009

Caplus now includes complete International Patent Classification (IPC) reclassification data for the third quarter of 2009.

CAS Information Use Policies apply and are available at:

<http://www.cas.org/legal/infopolicy.html>

This file contains CAS Registry Numbers for easy and accurate substance identification.

The ALL, BIB, MAX, and STD display formats in the CA/Caplus family of databases have been updated to include new citing references information. This enhancement may impact record import into database management software. For additional information, refer to NEWS 9.

=> s 13

L4 127 L3

=> s 14 py not > 2003

MISSING OPERATOR L4 PY

The search profile that was entered contains terms or nested terms that are not separated by a logical operator.

=> s 14 not py > 2003

7813375 PY > 2003

L5 82 L4 NOT PY > 2003

=> s 15 and ligand

374492 LIGAND

L6 0 L5 AND LIGAND

```

=> s 15 and affinity
    335097 AFFINITY
L7      1 L5 AND AFFINITY

=> s 15 and support
    579048 SUPPORT
L8      0 L5 AND SUPPORT

=> s 15 and solid
    1221171 SOLID
L9      2 L5 AND SOLID

=> s 15 and Fab
    19564 FAB
L10     0 L5 AND FAB

=> s 15 and IgG
    86381 IGG
L11     0 L5 AND IGG

=> s 15 and human
    2261058 HUMAN
L12     2 L5 AND HUMAN

=> s 15 and chromatography
    358201 CHROMATOGRAPHY
L13     0 L5 AND CHROMATOGRAPHY

=> s 15 and column
    470328 COLUMN
L14     0 L5 AND COLUMN

=> s 15 and matrix
    622387 MATRIX
L15     0 L5 AND MATRIX

=> s 15 and immunology
    6097 IMMUNOLOGY
L16     0 L5 AND IMMUNOLOGY

=> s 17 or 19 or 112
L17     5 L7 OR L9 OR L12

=> d 117 ibib abs hitstr 1-
YOU HAVE REQUESTED DATA FROM 5 ANSWERS - CONTINUE? Y/(N):y

```

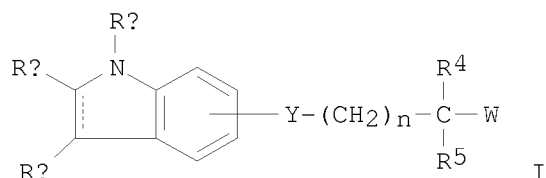
```

L17 ANSWER 1 OF 5  CAPLUS  COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER:      2002:449646  CAPLUS
DOCUMENT NUMBER:       137:33211
TITLE:                 Preparation of N-indolylurea derivatives as peroxisome
                        proliferator activated receptor  $\delta$  (PPAR  $\delta$ )
                        activators
INVENTOR(S):           Takahashi, Toshihiro; Sakuma, Shogo; Endo, Tsuyoshi;
                        Tendo, Atsushi; Yoshida, Shinichi; Kobayashi, Kunio;
                        Mochiduki, Nobutaka; Yamakawa, Tomio; Kanda, Takashi;
                        Masui, Seiichiro
PATENT ASSIGNEE(S):    Nippon Chemiphar Co., Ltd., Japan
SOURCE:                PCT Int. Appl., 81 pp.
                        CODEN: PIXXD2
DOCUMENT TYPE:         Patent
LANGUAGE:              Japanese
FAMILY ACC. NUM. COUNT: 1

```

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
WO 2002046154	A1	20020613	WO 2001-JP10576	20011204
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, US, UZ, VN, YU, ZA, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
AU 2002024138	A	20020618	AU 2002-24138	20011204
PRIORITY APPLN. INFO.:			JP 2000-369890	A 20001205
			WO 2001-JP10576	W 20011204
OTHER SOURCE(S):		MARPAT 137:33211		
GI				



AB Urea derivs. represented by the general formula (I) or salts thereof [wherein Y = O, S; n = an integer of 0-4; R₄, R₅ = H, C1-8 alkyl optionally substituted by 1-3 of halogen atoms; W = CO₂H, C2-8 alkoxy-carbonyl, SO₃H, cyano, tetrazolyl; a solid line accompanied by a dotted line represents a single or double bond; one of R_a, R_b, and R_c is R₁N(R₂)CON(R₃)X and the other two groups are H, C1-8 alkyl, C6-10 aryl, C1-8 alkyl-C6-10 aryl; wherein R₁, R₂, R₃ = H, C1-8 alkyl optionally substituted by 1-3 of halogen atoms, C1-8 alkoxy-C1-8 alkyl, C2-8 alkenyl, C2-8 alkynyl, C3-7 cycloalkyl, C3-7 cycloalkyl-C1-8 alkyl, C6-10 aryl, C6-10 aryl-C1-8 alkyl, heterocyclyl, heterocyclyl-C1-8 alkyl; X = C1-8 alkylene, remaining two R₈ and R₉ are each hydrogen or C1-8 alkyl; aryl, heterocyclyl, or aryl or heterocyclyl of arylalkyl or heterocyclylalkyl group is optionally substituted in R_a, R_b, and R_c] are prepared. These compds. are useful as blood sugar-lowering agents, hypolipidemics, antiobesity agents, hypocholesteremics, antiarteriosclerotics, anticancer agents, antiinflammatory agents, etc. Thus, 47 mg 2,4-dichlorophenyl isocyanate was added to a solution of 78 mg 2-[[1-[2-(isobutylamino)ethyl]indol-5-yl]oxy]-2-methylpropionic acid Et ester in EtOAc and stirred at room temperature for 0.5 h to give 83% 2-[[1-[2-(N'-2,4-dichlorophenyl-N-isobutylamino)ethyl]indol-5-yl]oxy]-2-methylpropionic acid Et ester which (96 mg) was dissolved in ethanol, treated with 1 M aqueous NaOH, stirred at room temperature for 16 h, treated with 0.1 M aqueous HCl under ice-cooling, and stirred at room temperature for 1 h to give 100% 2-[[1-[2-(N'-2,4-dichlorophenyl-N-isobutylureido)ethyl]indol-5-yl]oxy]-2-methylpropionic acid (II). In an assay for activating effect of PPAR δ receptor using CV-1 cells transfected with PPAR δ receptor-expressing plasmid, luciferase-expressing plasmid, and β -galactosidase-expressing plasmid, II at 10⁻⁵ M exhibited 106% activation compared to L-165041.

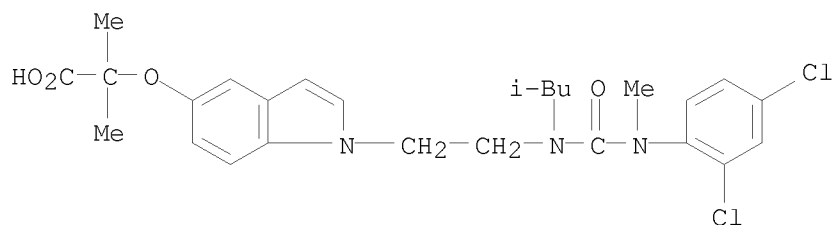
IT 435277-48-8P
RL: PAC (Pharmacological activity); SPN (Synthetic preparation); THU

(Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(preparation of N-indolylurea derivs. as peroxisome proliferator activated receptor δ (PPAR δ) activators for drugs)

RN 435277-48-8 CAPLUS

CN Propanoic acid, 2-[[1-[2-[[[(2,4-dichlorophenyl)methylamino]carbonyl](2-methylpropyl)amino]ethyl]-1H-indol-5-yl]oxy]-2-methyl- (CA INDEX NAME)



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD (3 CITINGS)
REFERENCE COUNT: 20 THERE ARE 20 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 2 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 2002:175776 CAPLUS

DOCUMENT NUMBER: 137:279130

TITLE: Identification of a novel, orally bioavailable histamine H3 receptor antagonist based on the 4-benzyl-(1H-imidazol-4-yl) template

AUTHOR(S): Aslanian, Robert; Mutahi, Mwangi W.; Shih, Neng-Yang; McCormick, Kevin D.; Piwinski, John J.; Ting, Pauline C.; Albanese, Margaret M.; Berlin, Michael Y.; Zhu, Xiaohong; Wong, Shing-Chun; Rosenblum, Stuart B.; Jiang, Yueheng; West, Robert; She, Susan; Williams, Shirley M.; Bryant, Matthew; Hey, John A.

CORPORATE SOURCE: The Schering Plough Research Institute, Kenilworth, NJ, 07033, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (2002), 12(6), 937-941

CODEN: BMCLE8; ISSN: 0960-894X

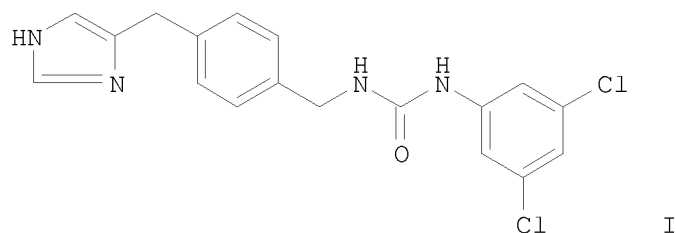
PUBLISHER: Elsevier Science Ltd.

DOCUMENT TYPE: Journal

LANGUAGE: English

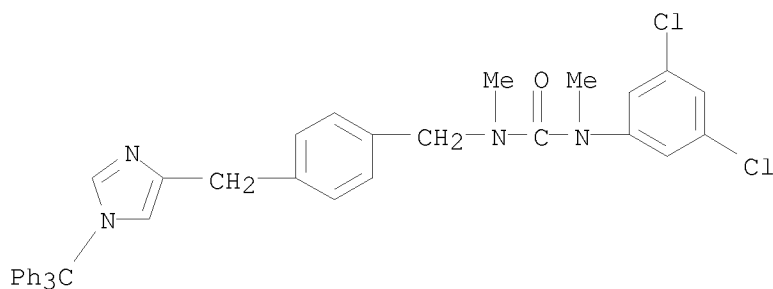
OTHER SOURCE(S): CASREACT 137:279130

GI

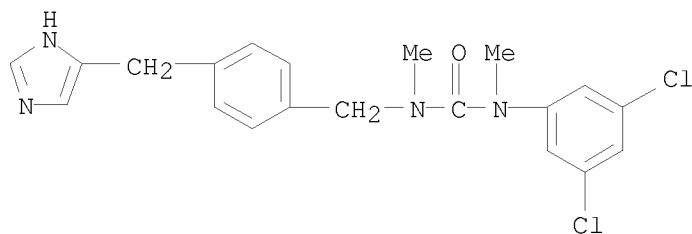


AB A novel series of histamine H3 receptor antagonists, based on the 4-benzyl-(1H-imidazole-4-yl) template, incorporating urea and carbamate linkers has been prepared. The urea I is a selective H3 antagonist and demonstrates excellent oral plasma levels in the rat and monkey.

IT 466671-37-4P
 RL: PAC (Pharmacological activity); SPN (Synthetic preparation); BIOL
 (Biological study); PREP (Preparation)
 (preparation of imidiazolymethylbenzylureas as histamine H3 receptor
 antagonists)
 RN 466671-37-4 CAPLUS
 CN Urea, N-(3,5-dichlorophenyl)-N,N'-dimethyl-N'-[[4-[[1-(triphenylmethyl)-1H-
 imidazol-4-yl]methyl]phenyl]methyl]- (CA INDEX NAME)



IT 705264-28-4P
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation of imidiazolymethylbenzylureas as histamine H3 receptor
 antagonists)
 RN 705264-28-4 CAPLUS
 CN Urea, N-(3,5-dichlorophenyl)-N'-[[4-(1H-imidazol-5-ylmethyl)phenyl]methyl]-
 N,N'-dimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 24 THERE ARE 24 CAPLUS RECORDS THAT CITE THIS
 RECORD (24 CITINGS)
 REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS
 RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 3 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2001:237842 CAPLUS
 DOCUMENT NUMBER: 134:266205
 TITLE: Preparation of collagen formation-inhibiting benzene
 derivatives
 INVENTOR(S): Kojima, Hiroshi; Sakamoto, Makoto; Yasumura, Koichi
 PATENT ASSIGNEE(S): Ohtsuka Pharmaceutical Co., Ltd., Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 97 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: Patent
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2001089412	A	20010403	JP 1999-269015	19990922

PRIORITY APPLN. INFO.:

JP 1999-269015

19990922

OTHER SOURCE(S):

MARPAT 134:266205

AB (R1)aC6H5-aVBWA [I; R1 = H, halo, OH, NO₂, cyano, etc.; a = 1-5; V = NHCO, CONH, NHCONH, NHC(S)NH, SCH₂CONH, etc.; B = p-C₆H₄, (un)substituted pyridine-2,5-diyl, pyrimidine-2,5-diyl, pyrazine-2,5-diyl, pyridine-2,3-diyl; W = O, S, SO, NH, CO, CH₂, SO₂; A = aryl] or their salts, useful for treatment of lung or liver fibrosis, are prepared
3,4,5-Trimethoxybenzoic acid (440 mg) was amidated by 500 mg
3-amino-6-(4-tert-butylphenoxy)pyridine in the presence of
1-ethyl-3-(3-dimethylaminopropyl)carbodiimide.HCl and
1-hydroxybenzotriazole in DMF at room temperature for 1 day to give 750 mg I
[(R1)a = 3,4,5-(OMe)₃, V = CONH, B = pyridine-2,5-diyl, W = O, A = C₆H₄CMe₃-p]. I [(R1)a = 3,4-Cl₂, V = CONH, B = p-C₆H₄, W = O, A = 5-oxo-5,6,7,8-tetrahydronaphthalen-1-yl] in vitro inhibited TGF
β-1-induced collagen synthesis in human LI90 cells with
IC₅₀ of 2.37 μM.

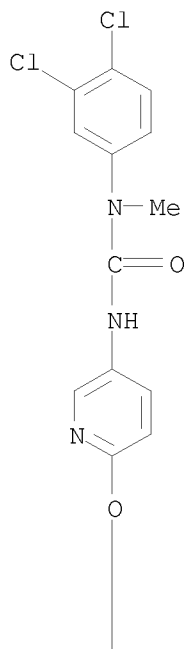
IT 332009-21-9P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation of collagen formation-inhibiting benzene derivs.)

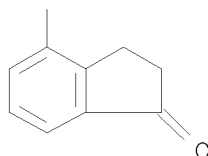
RN 332009-21-9 CAPLUS

CN Urea, N-(3,4-dichlorophenyl)-N'-[6-[(2,3-dihydro-1-oxo-1H-inden-4-yl)oxy]-3-pyridinyl]-N-methyl- (CA INDEX NAME)

PAGE 1-A



PAGE 2-A



OS.CITING REF COUNT: 3 THERE ARE 3 CAPLUS RECORDS THAT CITE THIS RECORD
(3 CITINGS)

L17 ANSWER 4 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1998:66714 CAPLUS

DOCUMENT NUMBER: 128:136098

ORIGINAL REFERENCE NO.: 128:26594h,26595a

TITLE: A Novel Class of Orally Active Non-Peptide Bradykinin
B2 Receptor Antagonists. 1. Construction of the Basic
Framework

AUTHOR(S): Abe, Yoshito; Kayakiri, Hiroshi; Satoh, Shigeki;
Inoue, Takayuki; Sawada, Yuki; Imai, Keisuke; Inamura,
Noriaki; Asano, Masayuki; Hatori, Chie; Katayama,
Akira; Oku, Teruo; Tanaka, Hirokazu

CORPORATE SOURCE: Exploratory Research Laboratories, Fujisawa
Pharmaceutical Co., Ibaraki, 300-26, Japan

SOURCE: Journal of Medicinal Chemistry (1998), 41(4), 564-578
CODEN: JMCMAR; ISSN: 0022-2623

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

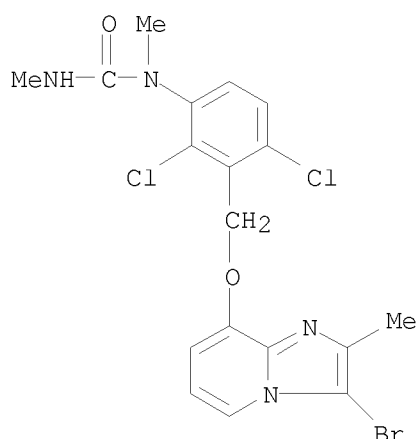
AB A novel class of potent, selective, and orally active non-peptide
bradykinin (BK) B2 receptor antagonists were designed and synthesized
starting from 8-benzyloxyimidazo[1,2-a]pyridine derivative(I). The unique
screening lead I was discovered by a 2-step intentional random screening
process, involving recognition of the relationship between BK and
angiotensin II (Ang II) and the common structural features. Systematic
chemical modification of I elucidated the structural requirements essential
for B2 binding affinity leading to the identification of
8-[[3-(N-acylglycyl-N-methylamino)-2,6-dichlorobenzyl]oxy]-3-halo-2-
methylimidazo[1,2-a]pyridine skeleton as the basic framework of this new
series of B2 antagonists. A mol. modeling study suggested the key role of
the N-methylanilide moiety at the 3-position of the 2,6-dichlorobenzene
ring to allow these compds. to adopt the characteristic active
conformation. The representative lead compds. inhibited the specific
binding of [3H]BK to guinea pig ileum membrane prepns. expressing B2
receptors, with nanomolar IC50s and also displayed in vivo functional
antagonistic activities against BK-induced bronchoconstriction in guinea
pigs at an oral dose of 1 mg/kg. Pharmacokinetic studies of the
N-butylamide and Et urea moieties at the 3-position of the
2,6-dichlorobenzene in rats highlighted their excellent oral
bioavailabilities, indicating that they represent the first orally active
non-peptide B2 antagonists reported to date.

IT 160642-24-0P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological
study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
BIOL (Biological study); PREP (Preparation); USES (Uses)
(preparation and MSBAR of nonpeptide bradykinin B2 receptor antagonists)

RN 160642-24-0 CAPLUS

CN Urea, N-[3-[[3-bromo-2-methylimidazo[1,2-a]pyridin-8-yl)oxy]methyl]-2,4-
dichlorophenyl]-N,N'-dimethyl- (CA INDEX NAME)



OS.CITING REF COUNT: 69 THERE ARE 69 CAPLUS RECORDS THAT CITE THIS
RECORD (70 CITINGS)
REFERENCE COUNT: 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS
RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L17 ANSWER 5 OF 5 CAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1967:508325 CAPLUS
DOCUMENT NUMBER: 67:108325
ORIGINAL REFERENCE NO.: 67:20403a,20406a
TITLE: Tuberculostatic urea derivatives
INVENTOR(S): Gagneux, Andre R.; Frick, Wilhelm
PATENT ASSIGNEE(S): Geigy, J. R., A.-G.
SOURCE: Ger., 5 pp.
CODEN: GWXXAW
DOCUMENT TYPE: Patent
LANGUAGE: German
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
DE 1246722		19670810	DE 1966-G48486	19661117
CH 456570			CH	
FR 1504098			FR	
FR 6433			FR	
GB 1125559			GB	
US 3539626		19701110	US	19681212
US 3621040		19710000	US	
US 3621100		19711116	US	19681118
PRIORITY APPLN. INFO.:			CH	19651118

AB The title compds. are prepared by treating a) adamantylamines with an aryl isocyanate, aryl isothiocyanate, or a carbanilic or thiocarbanilic acid derivative; b) an adamantyl isocyanate, isothiocyanate, carbamate, or thiocarbamate with an aryl amine; or c) an adamantyl and aryl substituted carbodiimide with H₂O or H₂S. Thus, a mixture of 36.5 millimoles 1-adamantylamine in 100 ml. absolute C₆H₆ and 33.3 millimoles 3,4-dichlorophenyl isocyanate in 100 ml. absolute C₆H₆ is heated at 80° 1 hr. and cooled and the filtered solid stirred 1 hr. in 100 ml. N HCl to give 1-(1-adamantyl)-3-(3,4-dichlorophenyl)urea, m. 220-1°. Similarly prepared are the following substituted 1-(1-adamantyl)ureas (substituents and m.p. given): 3-(p-MeC₆H₄), 252-6°; 3-(p-ClC₆H₄), 242-3°; 3-(2,4-Cl₂C₆H₃), 221-2°; 3-[6,3-Cl(F3C)C₆H₃], 233-4°; 3-(o-MeOC₆H₄), 234-6°; 3-(p-MeOC₆H₄), 235-8°; 3-[2,5(MeO)2C₆H₃], 240-2°; 3-(m-AcC₆H₄), 200-4°; 1-Me-3-(3,4-Cl₂C₆H₃), 193-5°; 3-Me-3-(3,4-Cl₂C₆H₃), 180-2°. Also prepared are

1-(1-adamantyl)thioureas: 3-(p-ClC₆H₄), 172-3°; 3-(2,4-Cl₂C₆H₃), 181-3°; 3-[4,3-Cl(F3C)C₆H₃], 169-71°; and 3-(3,4-Cl₂C₆H₃) (I), 189-92°. Similarly prepared are 1-(1-adamantylmethyl)-3-(3,4-dichlorophenyl)urea, m. 189-91°; 1-(α -methyl-1-adamantylmethyl)-3-(3,4-dichlorophenyl)urea, m. 195-8°; 1-(tricyclo[4.3.1.1^{3,8}]undec-3-yl)-3-(3,4-dichlorophenyl)urea, m. 233-6°; and 1-(2-oxaadamant-1-yl)-3-(3,4-dichlorophenyl)urea, m. 208-10°. To a mixture of 15 millimoles I in 600 ml. absolute dioxane is added 50 millimoles anhydrous MgSO₄ and 120 millimoles PbO, the mixture stirred at 60° 15 hrs., cooled, and filtered, the filtrate taken to dryness in vacuo, the oily residue dissolved in 300 ml. pentane, the turbid solution filtered through C, and the filtrate concentrated to give 1-(1-adamantyl)-3-(3,4-dichlorophenyl)carbodiimide, m. 60-1° (pentane). A mixture of 50 millimoles bicyclo[3.3.1]nonane-3,7-dione and 50 millimoles PhCH₂NH₂ in 300 ml. tetrahydrofuran is refluxed 0.5 hr., cooled, and added with stirring to 100 millimoles LiAlH₄ in 100 ml. absolute Et₂O, the mixture stirred at 40° 6 hrs., 19 ml. N NaOH added with ice-cooling, the precipitate filtered off, the filtrate evaporated, the residue dissolved in 500 ml. Me₂CO, and 5 ml. concentrated HCl added, to afford N-benzyl-2-oxaadamantylamine - HCl (II), m. 242-5°. A solution of 33 millimoles II in 100 ml. EtOH is hydrogenated with 50 atmospheric H in the presence of 2 g. 5% Pd-C at 100° 2 hrs., the mixture cooled and filtered, the filtrate evaporated, 25 ml. concentrated NaOH solution added to

the

residue, the mixture extracted with Et₂O, the Et₂O evaporated, and the residue sublimed at 60° and 0.1 mm. to yield 2-oxaadamantylamine, m. 148-54°; hydrochloride m. 280°.

IT 16192-94-2P

RL: SPN (Synthetic preparation); PREP (Preparation)
(preparation of)

RN 16192-94-2 CAPLUS

CN Urea, N-(3,4-dichlorophenyl)-N-methyl-N'-tricyclo[3.3.1.1^{3,7}]dec-1-yl-
(CA INDEX NAME)

